

Energy as an entanglement witness for quantum many-body systems

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We investigate quantum many-body systems where all low-energy states are entangled. As a tool for quantifying such systems, we introduce the concept of the *entanglement gap*, which is the difference in energy between the ground-state energy and the minimum energy that a separable (unentangled) state may attain. If the energy of the system lies within the entanglement gap, the state of the system is guaranteed to be entangled. We find Hamiltonians that have the largest possible entanglement gap; for a system consisting of two interacting spin-1/2 subsystems, the Heisenberg antiferromagnet is one such example. We also introduce a related concept, the *entanglement-gap temperature*: the temperature below which the thermal state is certainly entangled, as witnessed by its energy. We give an example of a bipartite Hamiltonian with an arbitrarily high entanglement-gap temperature for fixed total energy range. For bipartite spin lattices we prove a theorem demonstrating that the entanglement gap necessarily decreases as the coordination number is increased. We investigate frustrated lattices and quantum phase transitions as physical phenomena that affect the entanglement gap.

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I. INTRODUCTION

Understanding and quantifying the properties of quantum many-body systems is a central goal of theoretical condensed matter physics. Progress is often hindered by an incomplete understanding of the highly nonclassical entangled states that occur naturally as the ground and thermal states of many systems. Entanglement is perhaps the most counterintuitive feature of quantum mechanics and results in stronger correlations than can be present in any classical system [1,2]. Recently, entanglement has been recognized as an important resource in the emerging field of quantum information science [3], which has led to new tools that may enhance our understanding of the role of entanglement in quantum many-body systems.

Much recent work has focused on quantifying the entanglement naturally present in the ground state of standard models of coupled quantum systems, particularly spin chains. In [4–10] the role of entanglement in a *quantum phase transition* [11] is investigated. In one-dimensional chains, the amount of entanglement between a length of spins and the rest of the chain appears to depend only on the universality class of the model at the phase transition [6,7]. Various quantities associated with entanglement have been shown to display universal scaling behavior at phase transitions in one dimension [4,5,8]. Also, it appears that properties of entanglement between spins, such as the entanglement length defined in [12], are sometimes able to characterize phases of the system better than any correlation length [13].

Restricting to many-body systems where each system interacts with only a finite local neighborhood (which we refer to as *local interactions*) very strongly constrains the quantum states that must be considered. For example, there exist quantum states that are far from the ground state of any

local-interaction Hamiltonian [14]. For finite systems with local interactions and an energy gap it was shown in [15] that there are strong bounds on both the correlations and entanglement in the ground state. The fact that local interactions strongly limit the entanglement that can occur for Hamiltonian systems with local interactions on a line or a plane has been used to develop new approximation schemes for simulating quantum dynamics [16–21]. There is now a large literature on the entanglement properties of the ground states of Hamiltonian systems; we refer the reader to [22–27] and references therein.

Although the ground state plays an essential role in understanding physical systems, at finite temperature it is the thermal state that is of the greatest interest. The nature of entanglement in the thermal state of condensed matter systems was first studied by Nielsen [28], who investigated how entanglement in the thermal state varied with temperature and other parameters of simple systems consisting of two coupled spins. Subsequent work has investigated similar questions for quantum many-body systems [29–35]. A recent experiment demonstrates that entanglement can affect thermodynamic properties of a system at high temperature [36].

Thus, it seems that many physical phenomena involving just the ground or thermal states in condensed matter systems may be associated with the nature of entanglement in the system, and it is important to investigate new techniques for understanding and quantifying the role of entanglement in such systems. Desirable features of these techniques include that they be easily computable, even for large systems, that they be applicable at finite temperature, and that they be in principle easy to measure and related to known physics. Because most quantum systems are described by mixed states, these criteria lead naturally to the theory of mixed state entanglement.

Surprisingly, even the question of whether a mixed state of a quantum system is entangled or not is a difficult and much studied question. We refer the reader to the many reviews for the literature on the so-called separability problem

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[37–39]. The difficulty of this problem is one of the reasons why computing measures of entanglement can be so challenging and why it is important to find more tractable ways of understanding the entanglement in real physical systems. In this work we apply results from the theory of the separability problem to study the entanglement of quantum many-body systems. This investigation leads both to an understanding of the kind of Hamiltonians possessing strongly entangled thermal and low-energy states and also to interesting connections with properties of spin systems studied in more conventional condensed matter approaches.

The specific concept that we use from the theory of separability is that of an *entanglement witness*: an observable whose expectation value is positive if the state of interest is not entangled but for which a negative expectation value indicates that the state is entangled. An example of such an observable is the Bell observable which describes the outcomes of a test for the violation of Bell inequalities. In this paper we explore the idea of interpreting Hamiltonians with entangled ground states as entanglement witnesses. This point of view has attracted interest recently. During the preparation of this paper, related investigations appeared by Brukner and Vedral [40] and by Tóth [41] in which this type of entanglement witness is studied. As emphasized by Brukner and Vedral [40], because energy is a macroscopic thermodynamic property, it is reasonable to expect that it could be measured in experiment.

In this paper, we develop the idea of using energy as an entanglement witness for quantum many-body systems. We introduce two related concepts inspired by the theory of entanglement witnesses and discuss their relevance to both ground-state and finite-temperature properties of quantum many-body systems. The first is the *entanglement gap*: the difference in energy between the ground-state energy and the minimum energy that any separable (unentangled) state may attain. If the entanglement gap of a system is nonzero, then the entanglement of certain mixed states is detected simply by measuring their energy to be below this threshold. Roughly speaking, if the entanglement gap is small, then a separable state can be a good approximation to the ground state, and we expect approximation schemes based on separable states to produce reliable results. We investigate how large this gap can be for two-spin systems and how this gap depends on the coordination number for lattices of coupled spins.

One advantage of using ideas from studies of mixed-state entanglement is that it is possible to investigate systems at finite temperature. The second concept we introduce is the use of temperature as an indicator of entanglement in the thermal state. By comparing the thermal energy with the entanglement gap we obtain a temperature threshold, the *entanglement-gap temperature*, below which the thermal state is certainly entangled and we may expect entanglement to influence thermodynamic properties. We show that this temperature can become arbitrarily large as the dimension of two interacting spins increases even if the energy range of the system is kept fixed.

We begin in Sec. II with the observation that Hamiltonians with entangled ground states may be viewed as entanglement witnesses. We introduce the notion of entangle-

ment gap and provide necessary and sufficient conditions for this gap to be nonzero. We construct a one-to-one mapping between Hamiltonians with nonzero entanglement gap and entanglement witnesses. We prove a theorem that identifies a set of Hamiltonians with the largest possible gap; for spin-1/2 particles, one such Hamiltonian is the Heisenberg antiferromagnet. We then formally define the entanglement-gap temperature and investigate conditions that lead to a high value of this temperature. Somewhat counterintuitively, the Hamiltonians with the largest entanglement gap do not have the largest entanglement-gap temperature in general.

In Sec. III we study the entanglement gap in many-body systems, in particular spin models on lattices. We prove a general result that the entanglement gap must go to zero with increasing coordination number on a bipartite lattice with a fixed local interaction. This result is suggestive of a relationship to the success of mean-field theory on lattices with high coordination number. In Sec. IV, we conclude by investigating the dependence of the entanglement gap on frustration for the Heisenberg antiferromagnet. We show that for such systems it is possible to determine that the system is entangled even when the reduced state of nearest-neighbor spins is not entangled. We also investigate how the entanglement gap behaves near the quantum phase transition in the XY model and discuss its relationship to previous studies of entanglement at this transition.

II. HAMILTONIANS AS ENTANGLEMENT WITNESSES

In this section we establish a formal connection between Hamiltonians with the property that all low-energy states up to a certain energy are entangled and entanglement witnesses.

A multipartite mixed state of n subsystems is said to be *separable* if it can be expressed as a convex combination of pure product states:

$$\rho = \sum_i p_i |\psi_i^1\rangle\langle\psi_i^1| \otimes |\psi_i^2\rangle\langle\psi_i^2| \otimes \cdots \otimes |\psi_i^n\rangle\langle\psi_i^n|, \quad (1)$$

where $|\psi_i^j\rangle$ are pure states in the Hilbert space \mathcal{H}_j of subsystem j and $p_i > 0$, $\sum_i p_i = 1$. If a state can be decomposed in this way, then all correlations are purely classical; if not, then there exist truly quantum correlations and we say that the state is *entangled*.

An entanglement witness Z_{EW} on a multipartite system is a Hermitian operator (observable) with the properties that its expectation value in any separable state is greater than or equal to zero,

$$\text{tr}[Z_{EW}\rho_{\text{sep}}] \geq 0, \quad \forall \rho_{\text{sep}} \in \mathcal{S}, \quad (2)$$

where \mathcal{S} is the set of all separable states, and that there exists an entangled state ρ_{ent} such that

$$\text{tr}[Z_{EW}\rho_{\text{ent}}] < 0. \quad (3)$$

We say that Z_{EW} witnesses the entanglement of ρ_{ent} .

For a multipartite Hamiltonian H , we define the *minimum separable energy*

$$E_{\text{sep}} = \min_{\rho_{\text{sep}} \in \mathcal{S}} \text{tr}[H\rho_{\text{sep}}]. \quad (4)$$

Due to the convexity of the set of separable states, this minimum can always be achieved by a pure separable state. Note that there may be many separable states achieving this minimum separable energy E_{sep} .

If E_{sep} is strictly greater than the ground-state energy E_0 , there is a finite energy range over which all states are entangled. We refer to the size of this energy range as the entanglement gap.

Definition. For any multipartite Hamiltonian H , we define the *entanglement gap*

$$G_E = E_{\text{sep}} - E_0, \quad (5)$$

where E_0 is the ground-state energy of H . The entanglement gap is the energy gap between the ground-state energy and the minimum energy that a separable state can attain.

If H has an entangled nondegenerate ground state $|E_0\rangle$, then any separable state written in terms of the eigenstates of the Hamiltonian must contain contributions from higher-energy states and must therefore have higher energy than E_0 . If the ground state is degenerate, the same argument requires that the entanglement gap be greater than zero if there is no state in the ground-state manifold that is a pure product state. Conversely a nonzero entanglement gap requires that $E_{\text{sep}} > E_0$ and so there can be no pure product state in the ground-state manifold because such a state would have energy E_0 . So whether or not the entanglement gap is zero depends only on the ground-state manifold. *A Hamiltonian H has a nonzero entanglement gap if and only if no ground state of H is separable.*

Constructing Hamiltonians with a nonzero entanglement gap is straightforward. Every entanglement witness can be regarded as a Hamiltonian for a multipartite quantum system. For such Hamiltonians, $E_{\text{sep}}=0$ and E_0 is the minimum eigenvalue of Z_{EW} . The definition of entanglement witnesses implies that $E_0 < 0$ and thus the entanglement gap is nonzero.

Every Hamiltonian with a positive entanglement gap $G_E > 0$ defines an entanglement witness

$$Z_{EW} = H - E_{\text{sep}}I, \quad (6)$$

where I is the identity on the total Hilbert space. Because E_{sep} is the lowest possible energy for a separable state, we have $\text{tr}[Z_{EW}\rho_{\text{sep}}] = \text{tr}[H\rho_{\text{sep}}] - E_{\text{sep}} \geq 0$. On the other hand, if ρ_0 is a state in the ground-state manifold, we have $\text{tr}[Z_{EW}\rho_{\text{sep}}] = E_0 - E_{\text{sep}} < 0$, so Z_{EW} is an entanglement witness. Note that if H' and H differ only by an additive constant, they lead to the same entanglement witness. We regard such Hamiltonians as equivalent.

In summary, *there is a one-to-one map between entanglement witnesses and the equivalence classes of Hamiltonians with nonzero entanglement gap.*

The entanglement gap quantifies the range of energies over which all states are necessarily entangled. Note, however, that higher-energy states may still be entangled. So, for example, the thermal state for H must be entangled for all

temperatures such that the thermal energy is below E_{sep} but at higher temperatures the thermal state may or may not be entangled.

In Appendix A we describe an efficient numerical procedure, a sequence of semidefinite programs, for evaluating the entanglement gap and discuss the concept of bound entanglement in this context.

A. Hamiltonians that maximize the entanglement gap

Having defined the entanglement gap it is natural to identify Hamiltonians that have the largest possible entanglement gap for a given multipartite quantum system. We proceed by proving two lemmas: one that the entanglement gap is invariant under local unitary transformations of the Hamiltonian and the other regarding the optimal arrangement of the energy levels. We use these two lemmas to prove the main theorem of this section, which is that a set of Hamiltonians with maximum possible entanglement gap are those with a nondegenerate maximally entangled ground state and all other eigenstates at equal energy.

Lemma 1. Given a multipartite Hamiltonian H and a local unitary $U_{\text{local}} = U_1 \otimes U_2 \otimes \cdots \otimes U_N$ acting on each subsystem, the Hamiltonian $H' = U_{\text{local}} H U_{\text{local}}^\dagger$ has the same entanglement gap as H .

Proof. From the cyclic property of the trace, we have $\text{tr}[H'\rho'_{\text{sep}}] = \text{tr}[H\rho_{\text{sep}}]$, where $\rho_{\text{sep}} = U_{\text{local}}^\dagger \rho'_{\text{sep}} U_{\text{local}}$ is also separable. That is, for each ρ_{sep} with a certain energy under H there is a separable state ρ'_{sep} with the same energy under H' . Therefore $E_{\text{sep}} = E'_{\text{sep}}$. Also, because H and H' are related by conjugation by a unitary, they have the same spectrum and, in particular, the same ground-state energy. Hence H and H' have equal entanglement gap. ■

We now determine which Hamiltonians have the largest entanglement gap. For a comparison of gaps to be sensible, we need to scale by the overall energy range of the system. We define the *scaled entanglement gap* g_E as

$$g_E = G_E/E_{\text{tot}}, \quad (7)$$

where $E_{\text{tot}} = E_{\text{max}} - E_0$ is the total energy range and E_{max} is the highest energy eigenvalue.

Lemma 2. For any Hamiltonian with scaled entanglement gap g_E , the Hamiltonian $H' = I - |E_0\rangle\langle E_0|$, where $|E_0\rangle$ is a ground state for H , has a scaled entanglement gap g'_E greater than or equal to g_E .

Proof. We scale the Hamiltonian so that its lowest eigenvalue is zero and its highest eigenvalue is one, and thus the energy eigenvalues lie in the range $0 \leq E_i \leq 1$, $i=0, \dots, d_T - 1$, where d_T is the dimension of the total Hilbert space. The entanglement gap G_E of the scaled Hamiltonian \bar{H} is equal to the scaled entanglement gap g_E of the original Hamiltonian H . Note that the Hamiltonian H' is already scaled in this manner—i.e., $g'_E = G'_E$.

To prove the lemma, it is sufficient to show the stronger result $\text{tr}[\bar{H}\rho] \leq \text{tr}[H'\rho]$, $\forall \rho$; i.e., all states have higher energy under H' than under \bar{H} . To this end,

$$\mathrm{tr}[\rho \bar{H}] = \sum_{i=0}^{d_I-1} E_i \langle E_i | \rho | E_i \rangle \leq \sum_{i=1}^{d_I-1} \langle E_i | \rho | E_i \rangle = \mathrm{tr}[H' \rho], \quad (8)$$

as required. The inequality follows from the assumed range of energies $0 \leq E_i \leq 1 \forall i$ (where $E_0=0$) and the fact that $0 \leq \langle \psi | \rho | \psi \rangle \leq 1$ for any density operator ρ and any state $|\psi\rangle$ (because $0 \leq \rho \leq I$). Therefore E'_{sep} is necessarily greater than E_{sep} (even if the minimum-energy separable states are different), and because $E'_0=E_0=0$ and both Hamiltonians are scaled appropriately, we have $g'_E \geq g_E$, as required. ■

Using the geometric measure of entanglement for multipartite systems defined in [42], we consider multipartite pure states that are maximally entangled in the sense that they have *minimal* overlap with any pure product state—i.e., that they maximize the entanglement measure

$$M(|\Psi\rangle) = 1 - \max_{\rho_{\mathrm{sep}} \in \mathcal{S}} \langle \Psi | \rho_{\mathrm{sep}} | \Psi \rangle. \quad (9)$$

Let $M^{\max} = M(|\Psi_{\mathrm{me}}\rangle)$ be the maximum value of this measure, achievable by a maximally entangled state $|\Psi_{\mathrm{me}}\rangle$.

Theorem 1. The largest possible scaled entanglement gap of a multipartite system is $g_E^{\max} = M^{\max}$ and can be achieved by any Hamiltonian of the form $H' = I - |\Psi_{\mathrm{me}}\rangle\langle\Psi_{\mathrm{me}}|$, where $|\Psi_{\mathrm{me}}\rangle$ is a maximally entangled state by the measure of Eq. (9).

Proof. The proof follows from the definition of the entanglement gap,

$$g_E = 1 - \max_{\rho_{\mathrm{sep}} \in \mathcal{S}} \langle E_0 | \rho_{\mathrm{sep}} | E_0 \rangle, \quad (10)$$

and from Lemma 2. ■

Although we do not present the result here, it is also possible to show [43] that all Hamiltonians that have this minimum entanglement gap are of this form.

For multipartite systems it is not known which states are maximally entangled according to the measure M . However, in [42] examples of highly entangled states are given, which place lower bounds on the maximum size of the scaled entanglement gap. For example, if each of the n subsystems are d dimensional, there exists a symmetrized state $|S(n, d)\rangle$ such that $M(|S(n, d)\rangle)$ approaches 1 as d^{-2n} in the $n \rightarrow \infty$ limit. If each of the n subsystems are n dimensional, there is an antisymmetrized state $|A(n)\rangle$ such that $M(|A(n)\rangle) = 1 - 1/n!$. It is clear that entanglement gap can be a very large fraction of the total energy range for large numbers of coupled systems.

Bipartite entanglement is much better understood than multipartite entanglement, and the following corollary gives an explicit form for the maximally entangled ground state and the corresponding maximum possible scaled entanglement gap for bipartite systems.

Corollary. The largest scaled entanglement gap for a bipartite system $\mathcal{H}_A \otimes \mathcal{H}_B$ is $g_E = 1 - 1/d$, where $d = \min(d_A, d_B)$ is the smaller dimension of the two subsystems and is achieved by any Hamiltonian of the form $H' = I - |\phi_d\rangle\langle\phi_d|$, where $|\phi_d\rangle = (1/\sqrt{d}) \sum_{i=1}^d |i_A\rangle |i_B\rangle$ and $\{|i_{A/B}\rangle\}$ are orthonormal bases for $\mathcal{H}_{A/B}$.

Proof. It follows from the convexity of the set of separable density matrices that the maximum overlap between a

pure ground state and a separable state is achieved by a *pure* product state $\rho_{\mathrm{sep}} = |A\rangle\langle A| \otimes |B\rangle\langle B|$, where $|A\rangle \in \mathcal{H}_A$, $|B\rangle \in \mathcal{H}_B$. In fact, the maximum is achieved by setting $|A\rangle = |1_A\rangle$, $|B\rangle = |1_B\rangle$,

$$\max_{\rho_{\mathrm{sep}} \in \mathcal{S}} \langle E_0 | \rho_{\mathrm{sep}} | E_0 \rangle = \lambda_1^2, \quad (11)$$

where the Schmidt decomposition [3] for $|E_0\rangle$ is $|E_0\rangle = \sum_{i=1}^d \lambda_i |i_A\rangle |i_B\rangle$ and λ_1 is the largest Schmidt coefficient.

Thus, the largest scaled entanglement gap results from finding $|E_0\rangle$ with the smallest possible λ_1 . Normalization ($\sum_i \lambda_i^2 = 1$) requires that $\lambda_1^2 \geq 1/d$ and $\lambda_1^2 = 1/d$ is achieved by any maximally entangled bipartite state $|E_0\rangle = |\phi_d\rangle$. Thus, the Hamiltonian $H = I - |\phi_d\rangle\langle\phi_d|$ achieves the maximum possible scaled entanglement gap $g_E = 1 - 1/d$. ■

For $d_A = d_B = 2$, the Hamiltonian $H = I - |\phi_2\rangle\langle\phi_2|$, where $|\phi_2\rangle = \sum_{i=1}^2 |i_A\rangle |i_B\rangle / \sqrt{2}$ is any maximally entangled state, has the largest entanglement gap. If the Hilbert space corresponds physically to two spin-1/2 systems, then a particularly enlightening example of a Hamiltonian of this form is a shifted and scaled version of the antiferromagnetic Hamiltonian, $H = \vec{\sigma}_A \cdot \vec{\sigma}_B$, where $\vec{\sigma}_i$, $i = A, B$, is the vector of Pauli matrices on \mathcal{H}_i . It is straightforward to show that

$$H = I - |\psi^-\rangle\langle\psi^-| = (\vec{\sigma}_A \cdot \vec{\sigma}_B + 3I)/4,$$

where $|\psi^-\rangle = (|0\rangle_A |1\rangle_B - |1\rangle_A |0\rangle_B) / \sqrt{2}$ is the singlet state.

B. Entanglement-gap temperature

In the following, we investigate the temperature at which the thermal state reaches the minimum separable energy. We find the temperature below which the thermal state is guaranteed to be entangled; this temperature also provides a non-trivial lower bound on the temperature above which the thermal state is guaranteed to be separable.

A quantum system with Hamiltonian H in thermal equilibrium at temperature T is described by the thermal state

$$\rho_T = \exp(-\beta H) / Z, \quad (12)$$

where $\beta = 1/k_B T$ is the inverse temperature, k_B is Boltzmann's constant, and $Z = \mathrm{tr}[\exp(-\beta H)]$ is the partition function. The energy of the thermal state, the *thermal energy*, is given by

$$U(T) = \mathrm{tr}[H \rho_T] = - \frac{1}{Z} \frac{\partial Z}{\partial \beta}. \quad (13)$$

Definition. Given a system with an entanglement gap greater than zero, $G_E > 0$, we define the *entanglement-gap temperature* T_E to be the temperature at which the thermal energy equals the minimum separable energy, $U(T_E) = E_{\mathrm{sep}}$.

The thermal energy is a monotonically decreasing function of β (i.e., it decreases as the temperature decreases). By definition, all states with energy less than E_{sep} are guaranteed to be entangled, and thus the system is certainly entangled below the entanglement-gap temperature. That is, if we cool our system down below the entanglement-gap temperature, we know it must be in an entangled state. The thermal energy of the system, which depends only on the temperature, be-

comes a witness to the entanglement of the thermal state.

In order to compare Hamiltonians with different total energy ranges E_{tot} , it is sensible to define a *scaled temperature* t as

$$t = k_B T / E_{\text{tot}}. \quad (14)$$

The corresponding *scaled entanglement-gap temperature* is $t_E = k_B T_E / E_{\text{tot}}$.

For the class of Hamiltonians identified in Theorem 1 with maximal entanglement gap—i.e., $H = I - |\Psi_{\text{me}}\rangle\langle\Psi_{\text{me}}|$, where $|\Psi_{\text{me}}\rangle$ is a maximally entangled state by the measure (9)—it is straightforward to calculate the entanglement-gap temperature. The thermal energy is given by

$$U(t) = \frac{(d_T - 1)\exp(-\beta)}{1 + (d_T - 1)\exp(-\beta)}. \quad (15)$$

Setting $U(t_E) = E_{\text{sep}} = M^{\text{max}}$ gives

$$t_E = \left[\log_e \frac{(d_T - 1)(1 - M^{\text{max}})}{M^{\text{max}}} \right]^{-1}. \quad (16)$$

As an example, we consider the entanglement-gap temperature of a bipartite system (each subsystem of dimension d), with Hamiltonian $H = I - |\phi_d\rangle\langle\phi_d|$ and scaled entanglement gap $g_E = 1 - 1/d$. The scaled entanglement-gap temperature for this system is

$$t_E = [\log_e(d + 1)]^{-1}. \quad (17)$$

Note that the entanglement-gap temperature decreases with increasing dimension despite the fact that the entanglement gap increases. This behavior is due to the fact that the number of eigenstates with energy one increases quadratically with d , while the ground state remains nondegenerate.

C. Hamiltonians of bipartite systems possessing large entanglement-gap temperature

It is natural to ask which Hamiltonians have the highest (scaled) entanglement-gap temperature. Somewhat counter-intuitively it is not the Hamiltonians with the largest entanglement gap. In fact, there are Hamiltonians with arbitrarily high entanglement-gap temperature. To provide an example, we restrict our attention to the case where the two subsystems of the bipartite system have the same dimension, $d_A = d_B = d$. The projectors onto the symmetric and antisymmetric subspaces of $\mathcal{H}_A \otimes \mathcal{H}_B$ are $\Pi_S = (I + V_{(A,B)})/2$ and $\Pi_A = (I - V_{(A,B)})/2$, respectively, where $V_{(A,B)}$ is the permutation operator on the two subsystems, defined by $V_{(A,B)}|\psi\rangle_A|\phi\rangle_B = |\phi\rangle_A|\psi\rangle_B$ for all $|\psi\rangle, |\phi\rangle$. The antisymmetric subspace contains only entangled states. Thus, if we define a Hamiltonian as the projector onto the symmetric subspace

$$H = \Pi_S, \quad (18)$$

then all symmetric states have energy 1, all antisymmetric states have energy 0, and there is a finite entanglement gap. We find the gap by directly calculating the energy of a pure separable state, $|A\rangle|B\rangle$,

$$\langle A|\langle B|H|A\rangle|B\rangle = (1 + |\langle A|B\rangle|^2)/2. \quad (19)$$

From this expression it is clear that the minimum energy of $1/2$ is achieved by any pure separable state such that $\langle A|B\rangle = 0$. The entanglement gap is $G_E = 1/2$, independent of d .

For the symmetric-projector Hamiltonian the thermal energy is given by

$$U(t) = \frac{d(d+1)\exp(-\beta)}{d(d-1) + d(d+1)\exp(-\beta)}. \quad (20)$$

Using $E_{\text{sep}} = 1/2$ we find

$$t_E = \left[\log_e \left(\frac{d+1}{d-1} \right) \right]^{-1} \simeq d/2 \quad \text{for } d \gg 1. \quad (21)$$

Remarkably, for this Hamiltonian the scaled entanglement-gap temperature increases without bound as the dimension of the subsystems increases.

Thus, for Hamiltonians that only have eigenvalues 0 or 1, there is a trade-off between ground-state degeneracy and the entanglement gap in determining the entanglement-gap temperature. Even though the Hamiltonian with a nondegenerate maximally entangled ground state has a larger entanglement gap, the symmetric-projector Hamiltonian has a higher entanglement-gap temperature due to its large ground-state degeneracy.

In Appendix B, we investigate other Hamiltonians with ground-state manifolds containing only entangled states and present evidence that no other bipartite Hamiltonian with a two-level energy spectrum possesses an entanglement-gap temperature greater than the Hamiltonian (18). In Appendix C, we investigate the entanglement temperature of two-qubit systems and provide evidence that the Heisenberg antiferromagnetic Hamiltonian has the highest entanglement-gap temperature.

We note that Tóth [41] gives an example of a multiparty Hamiltonian, the Heisenberg interaction between all pairs of n spin-1/2 particles, whose entanglement-gap temperature increases linearly with n ; i.e., it is arbitrarily high for arbitrarily large systems. However, unlike our example, the total energy range also increases linearly with n . The scaled entanglement-gap temperature of their Hamiltonian therefore approaches a constant as $n \rightarrow \infty$. By contrast, the entanglement-gap temperature of our example is arbitrarily high despite the fact that the total energy range is bounded.

III. ENTANGLEMENT GAP OF QUANTUM MANY-BODY SYSTEMS

In this section, we investigate the entanglement gap for quantum systems arranged on some graph or lattice that interact with some local neighborhood. Because we are only considering finite-dimensional systems, the subsystems can always be thought of as spins of some total angular momentum, so we use the terms “subsystem” and “spin” interchangeably. For a particular type of coupling—bipartite lattices—we provide an explicit method for calculating the entanglement gap, which applies to various spin systems of-

ten considered in the condensed matter literature. We also prove that, as the coordination number grows, the entanglement gap per interaction must decrease to zero. This result makes use of the fact that as the number of equivalent spins connected to a given spin in the lattice increases there does not exist a global state of the system for which each interacting pair is strongly entangled.

A. Entanglement gap of 2-local Hamiltonians

We now consider multipartite systems with only two-body interactions. The Hamiltonian for such a system can be defined by a set of coupling Hamiltonians H_{ij} that act as the identity on all the spins other than i and j and a graph or lattice where the vertices represent spins and edges represent an interaction between the spins on the two sites. We refer to each two-body interaction, or edge on the graph, as a *bond*. The Hamiltonian for the entire system is

$$H = \sum_{\langle i,j \rangle} H_{ij}, \quad (22)$$

where $\sum_{\langle i,j \rangle}$ indicates a sum over vertices connected by an edge—i.e., a sum over bonds. We refer to such a Hamiltonian as *2-local*. It follows that the energy of a 2-local Hamiltonian depends only on the reduced density matrices of each interacting pair; see, e.g., [10]. Thus, the energy for any global state ρ is

$$E = \text{tr}[H\rho] = \sum_{\langle i,j \rangle} \text{tr}[H_{ij}\rho_{ij}], \quad (23)$$

where ρ_{ij} is the reduced state of the interacting pair of spins $\langle i,j \rangle$. In the following we consider only systems where each of the coupling Hamiltonians H_{ij} is equal.

We note that the reduced states ρ_{ij} are not completely arbitrary if they are to be consistent with a global state ρ for the whole system. In particular, the ground state of the graph or lattice cannot simply be constructed from the reduced states that minimize the energy of each bond ($\text{tr}[H_{ij}\rho_{ij}]$), because these reduced states may not be consistent with a global state. As we demonstrate below, this situation can occur when there is a nonzero entanglement gap for the coupling Hamiltonian H_{ij} . Motivated by the results of Sec. II as well as its importance in condensed matter physics, we use the Heisenberg antiferromagnet as our standard example.

A *bipartite* graph or lattice is one for which the vertices can be divided into two sets A and B , such that the edges only connect vertices from A with vertices from B . Examples of bipartite lattices include the square lattice (see Fig. 1) and the hexagonal lattice on the plane. An even number of vertices arranged in a ring is also bipartite.

For bipartite graphs or lattices, we now demonstrate how to construct a separable state with the lowest possible energy. First, consider a minimum-energy separable state $|A\rangle|B\rangle$ for a pair of spins under the interaction Hamiltonian and construct a global state $\otimes_{i_A \in A} |A\rangle_{i_A} \otimes_{i_B \in B} |B\rangle_{i_B}$, such that all the spins on the subset A are in the state $|A\rangle$ and likewise for B . By Eq. (23) the energy per bond of this state is the same as the energy E_{sep} of the state $|A\rangle|B\rangle$, and it provides an upper bound on the minimum separable energy per bond of the full

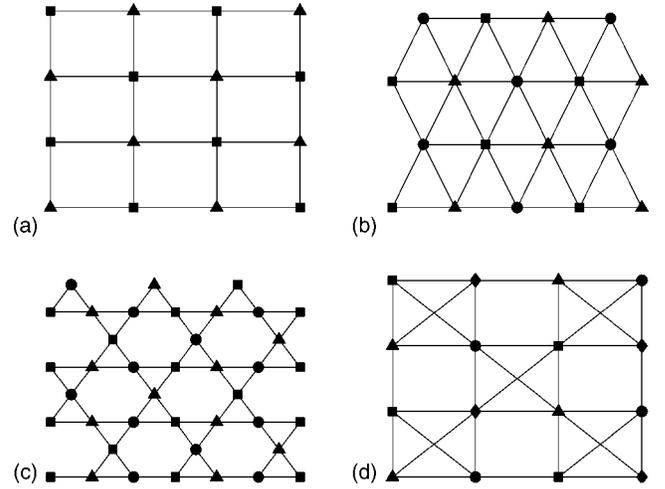


FIG. 1. Examples of n -partite lattices. (a) Square lattice ($n=2$), (b) triangular lattice ($n=3$), (c) kagomé lattice ($n=3$), and (d) checkerboard lattice ($n=4$). The n different markers indicate the n subsets that the vertices of the n -partite lattice may be divided into so that there are only interactions between distinct subsets.

Hamiltonian (22). To see that there is no global separable state with lower energy, suppose that such a state exists. Then all of the nearest-neighbor reduced density matrices ρ_{ij} must be separable and by Eq. (23) at least one of them must have a lower energy under the interaction Hamiltonian than $|A\rangle|B\rangle$: a contradiction. Therefore, the state $\otimes_{i_A \in A} |A\rangle_{i_A} \otimes_{i_B \in B} |B\rangle_{i_B}$ is indeed a minimum-energy separable state of the entire system.

Given this result, we can determine the lowest possible energy of a separable state for the Hamiltonian (22) on any bipartite graph or lattice simply by solving the problem for a single pair of spins. Finding the entanglement gap for such systems reduces to finding the entanglement gap of the two-body interaction and the ground-state energy E_0 of the overall system. This important fact was noted by Tóth [41] who provided a slightly different argument.

Consider a bipartite graph with Hamiltonian H . Then our argument proves that the operator $H - NE_{\text{sep}}$ is an entanglement witness, where N is the number of bonds. Note that we can express this entanglement witness as a sum over bonds,

$$H - NE_{\text{sep}} = \sum_{\langle i,j \rangle} (H_{ij} - E_{\text{sep}}), \quad (24)$$

where each term in the sum is a bipartite entanglement witness. As a result the expectation value depends only on the bipartite reduced density matrices of nearest neighbors and can only be negative if these reduced density matrices are entangled. This result can be extended to apply to lattices (with $N \rightarrow \infty$) as well. So, while the ground-state energy is certainly a global quantity, this construction is only sufficient to detect the existence of bipartite entanglement between interacting pairs in a bond.

In a similar way we can calculate the entanglement gap for n -partite graphs or lattices that are formed by groups of n spins each having an “all-to-all” interaction graph. We first construct a minimum-energy separable state of a single

group of n spins with an all-to-all interaction graph. This state extends to a minimum-energy separable state of the entire lattice as depicted in Fig. 1. We then compare the minimum-separable energy per bond to the ground-state energy per bond to find the entanglement gap per bond. For example, on the tripartite triangular and kagomé lattices (see Fig. 1), it is possible to calculate the entanglement gap from the ground-state energy and the minimum separable energy of three spins having an all-to-all interaction graph (a single triangle). We describe the nature of the entanglement that can be witnessed in these systems in Sec. IV B.

B. Entanglement gap and coordination number

The *coordination number* of a lattice is the number of edges incident on each lattice site—i.e., the number of other systems that each spin interacts with via the coupling Hamiltonian H_{ij} . As we are now considering lattices, our assumption that all interactions H_{ij} are equal implies translational symmetry. We now investigate how the entanglement gap varies with the coordination number of the lattice. The basic idea stems from the fact that, as a result of the translational symmetry, the ground states of our 2-local Hamiltonians have equal reduced density matrices for interacting pairs.¹ As the coordination number increases, this equality requires that every spin share the same reduced density matrix with an increasing number of other spins. The results of [44–46] then preclude the reduced density matrices from being strongly entangled. Building on these results, we prove a theorem stating that, as the coordination number of the lattice grows, the entanglement gap decreases to zero. We then investigate this behavior in the specific case of the Heisenberg antiferromagnet.

In order to prove results about the maximum possible entanglement gap in Sec. II A it was natural to use the scaled entanglement gap. However, in what follows it is more convenient to use the *entanglement gap per bond*, G_E/N , where N is the total number of bonds. (Note that this entanglement gap per bond is well defined even for lattices with $N \rightarrow \infty$.) These two methods of scaling are roughly equivalent because the total energy range of the system tends to scale linearly with the number of sites.

We begin by considering a restricted set of graphs which we will use to prove results that bound the entanglement gap on any bipartite lattice. We define a *star* graph as a bipartite graph where there is only a single vertex, the *center*, in one subset, $A = \{A_0\}$, and k vertices, the *points*, in the other subset, $B = \{B_i, i=0, \dots, k-1\}$, and where edges connect each point and the center.

A *strictly positive* entanglement witness Z_{EW} is a Hermitian operator whose average is strictly positive on separable states $\text{tr}[Z_{EW}\rho_{\text{sep}}] > 0$, $\forall \rho_{\text{sep}} \in \mathcal{S}$, but which has at least one negative eigenvalue.

Before stating and proving our main theorem we present the following lemma.

Lemma 3. Let Z_{EW} be a strictly positive entanglement wit-

ness acting on $\mathcal{H}_{A_0} \otimes \mathcal{H}_{B_0}$. Then there exists a positive integer k such that

$$\sum_{i=0}^{k-1} V_{(B_0, B_i)} (Z_{EW} \otimes_{i=1}^{k-1} I_{B_i}) V_{(B_0, B_i)}^\dagger \geq 0, \quad (25)$$

where $V_{(B_0, B_i)}$ is the self-adjoint unitary operator that swaps the Hilbert spaces \mathcal{H}_{B_0} and \mathcal{H}_{B_i} .

This lemma is a straightforward modification of Theorem 2 of [44] and the proof follows similarly.²

Using the general mapping between entanglement witnesses and Hamiltonians with nonzero entanglement gap discussed in Sec. II, this result on strictly positive entanglement witnesses bounds the entanglement gap for Hamiltonians on star graphs.

Theorem 2. For any coupling Hamiltonian $H_{A_0 B_0}$ and any $\epsilon > 0$ there exists a positive integer k such that the entanglement gap per interaction for the Hamiltonian (22) on a star graph with k points is less than ϵ .

Proof. The nontrivial case occurs when $H_{A_0 B_0}$ has nonzero entanglement gap. Note that the total Hamiltonian on the star graph may be written as

$$H^{\text{star}} = \sum_{i=0}^{k-1} V_{(B_0, B_i)} (H_{A_0 B_0} \otimes_{i=1}^{k-1} I_{B_i}) V_{(B_0, B_i)}^\dagger. \quad (26)$$

We define a strictly positive entanglement witness on $\mathcal{H}_{A_0} \otimes \mathcal{H}_{B_0}$ as

$$Z_{EW} = H_{A_0 B_0} - E_{\text{sep}} I + \epsilon I, \quad (27)$$

where E_{sep} is the energy of the minimum-energy separable state of $H_{A_0 B_0}$ and, by adding $\epsilon > 0$, Z_{EW} is guaranteed to be a strictly positive entanglement witness. From Lemma 3, there exists a k such that

$$\sum_{i=0}^{k-1} V_{(B_0, B_i)} [(H_{A_0 B_0} - E_{\text{sep}} + \epsilon) \otimes_{i=1}^{k-1} I_{B_i}] V_{(B_0, B_i)}^\dagger \geq 0,$$

and so $H^{\text{star}} \geq k(E_{\text{sep}} - \epsilon)$. Because the energy of the minimum-energy separable state of H^{star} is kE_{sep} , this implies that the entanglement gap of the total Hamiltonian satisfies $G_E^{\text{star}} \leq k\epsilon$. Thus, given any $\epsilon > 0$ there exists a k such that $G_E^{\text{star}}/k \leq \epsilon$, as claimed. ■

As an illustration of this theorem we consider the spin-1/2 Heisenberg antiferromagnetic Hamiltonian on a star graph. Recall that the coupling Hamiltonian is $H_{ij} = \vec{\sigma}_i \cdot \vec{\sigma}_j$; the entanglement gap of this coupling Hamiltonian was investigated in Sec. II A. The ground state is the singlet, with energy -3 , and the three triplet states all have energy $+1$. The minimum-energy separable states are of the form $|A\rangle|B\rangle$ such that $\langle A|B\rangle = 0$, with energy -1 .

²The key difference between this proof and the one found in [44] is that, here, mixing with the operators $V_{(B_0, B_i)}$ forces the resulting entanglement witness to be block diagonal in the irreducible representations of the symmetric group, rather than projecting into the fully symmetric representation of this group as in [44].

¹If there is spontaneous symmetry breaking, a mixture of the symmetry-broken ground states will be translationally invariant.

TABLE I. Properties of star graphs with the Heisenberg antiferromagnetic Hamiltonian as a function of coordination number k . The ground-state energy, minimum separable energy, and entanglement gap are all *per bond*—i.e., energies divided by k . The scaled entanglement gap is the entanglement gap divided by the total energy range of the system.

| Coord. No. k | E_0 per bond | E_{sep} per bond | Ent. gap per bond | Scaled ent. gap |
|----------------|----------------|---------------------------|-------------------|-----------------|
| 1 | -3 | -1 | 2 | 0.5 |
| 2 | -2 | -1 | 1 | 0.333 |
| 3 | -1.667 | -1 | 0.667 | 0.25 |
| 4 | -1.5 | -1 | 0.5 | 0.2 |
| 5 | -1.4 | -1 | 0.4 | 0.167 |
| 6 | -1.333 | -1 | 0.333 | 0.143 |

Using the permutation symmetry amongst the points of the Hamiltonian on the star graph it is possible to calculate its ground-state energy exactly [47], $E_0 = -(k+2)$. The coordination number of the center of the graph is the number of points, k . The energy of any minimum-energy separable state is $E_{\text{sep}} = -k$. In Table I we present the entanglement gap per bond and the scaled entanglement gap for comparison with other lattices below.

Although the Heisenberg antiferromagnet has the largest entanglement gap for two qubits, we have not proved that it has the largest entanglement gap per bond on a star graph. However, we have calculated the entanglement gap per bond for numerous common spin models such as the XXZ model and XY model, all of which have a smaller entanglement gap per bond. Therefore we conjecture that the Heisenberg antiferromagnet has the largest entanglement gap per bond on a star graph. If this were true, it would provide an upper bound of $O(1/k)$ on the approach to zero of the entanglement gap per bond implied by Theorem 2.

In order to determine the entanglement gap on a bipartite lattice, we require the ground-state energy of the lattice as well as the lowest energy achievable by a separable state of a single pair of spins, as noted above. The ground-state energy of a star graph can be used to bound the ground-state energy of a bipartite lattice with the same coordination number as follows.

Lemma 4. The ground-state energy per bond of any coupling Hamiltonian on a bipartite lattice with coordination number k is greater than or equal to the ground-state energy per bond of the same Hamiltonian on a star graph with k points.

Proof. The essential idea is to divide the expression for ground-state energy on the lattice into a sum over star graphs with k points where k is the coordination number of the lattice. Let ρ_0 denote the translationally invariant ground state of the entire lattice. Consider the star graph consisting of a particular lattice site (the center) and those sites connected to it by a coupling (the points). The reduced state on the star graph is obtained by tracing out all sites not in the star:

$$\rho_{\text{star}} = \text{tr}_{i \notin \{\text{star}\}}[\rho_0]. \quad (28)$$

This state is independent of the lattice site chosen as the center (due to the translational invariance of ρ_0), and the energy per bond of this reduced state is the same as the ground-state energy per bond of the lattice. The ground-state energy is then

$$E_0 = \text{tr}[H\rho_0] = \sum_i \text{tr}[H_{\text{star}}\rho_{\text{star}}]/k. \quad (29)$$

Furthermore, the energy of ρ_{star} can only be greater than the energy of a ground state $|E_0\rangle_{\text{star}}$ of the star Hamiltonian:

$$\text{tr}[H_{\text{star}}\rho_{\text{star}}] \geq \text{tr}[H_{\text{star}}|E_0\rangle_{\text{star}}\langle E_0|]. \quad (30)$$

It follows that the ground-state energy per bond of the bipartite lattice is greater than or equal to the ground-state energy per bond of the star graph. ■

We note that a similar argument is used in [48] to bound the ground-state energy of the Heisenberg antiferromagnet.

Using this bound for the ground-state energy, it is straightforward to bound the entanglement gap on bipartite lattices, which is the main result of this section.

Theorem 3. Given any $\epsilon > 0$ there exists a positive integer k such that the entanglement gap per bond for an arbitrary coupling Hamiltonian on any bipartite lattice with coordination number k is less than ϵ .

Proof. Because the bipartite lattice and star graph are both bipartite, they have the same minimum separable energy per bond. The result now follows from Theorem 2 and Lemma 4. ■

To illustrate this theorem, we calculate the entanglement gap per bond of the spin-1/2 Heisenberg antiferromagnet on simple bipartite lattices with varying coordination number. In Table II we present the ground-state energy, taken from the literature, and thus the entanglement gap per bond and scaled entanglement gap for a Heisenberg antiferromagnet on a one-dimensional (1D) chain, honeycomb, square, and cubic lattice (all bipartite), as well as some nonbipartite lattices to be discussed in Sec. IV B. It can be seen that the entanglement gap per bond does decrease with increasing coordination number for the bipartite case and is always less than that of the corresponding star graph in Table I, as proved by Lemma 4. The entanglement gap per bond appears to decrease with coordination number on tripartite lattices as well, thus providing evidence that this behavior is not confined to bipartite lattices.

IV. DISCUSSION

In this section, we discuss some of the implications of our results and explore the connections with other results from the condensed matter literature. We also discuss frustrated lattices and quantum phase transitions and their effect on the entanglement gap.

The energy gap between the ground-state energy and the lowest energy achieved by a separable state has been discussed in the quantum magnetism literature using a slightly different terminology [49]. There, separable states are associated with “classical configurations,” arrangements of clas-

TABLE II. Entanglement gap for the Heisenberg antiferromagnet for various bipartite and frustrated lattices with different coordination numbers. Ground-state energies taken from [49].

| Lattice | Coord. No. | E_0 per bond | E_{sep} per bond | Ent. gap per bond | Scaled ent. gap |
|--------------------|------------|---------------------|---------------------------|-------------------|-----------------|
| Single bond | 1 | -3 | -1 | 2 | 0.5 |
| 1D chain | 2 | -1.772 | -1 | 0.772 | 0.279 |
| Hexagonal | 3 | -1.452 | -1 | 0.452 | 0.184 |
| Square | 4 | -1.338 | -1 | 0.338 | 0.145 |
| Cubic | 6 | -1.194 ^a | -1 | 0.194 | 0.088 |
| Single triangle | 2 | -1 | -0.5 | 0.5 | 0.25 |
| Kagomé | 4 | -0.874 | -0.5 | 0.374 | 0.200 |
| Triangular | 6 | -0.726 | -0.5 | 0.226 | 0.131 |
| Single tetrahedron | 3 | -1 | -0.333 | 0.667 | 0.333 |
| Checkerboard | 6 | -0.67 ^b | -0.333 | 0.34 | 0.20 |

^aFrom linear spin-wave theory [50].

^bFrom [51].

sical spin vectors minimizing the energy of the appropriate classical Heisenberg spin model. The reduction in ground-state energy below this point is typically ascribed to “quantum fluctuations.” As a result, Table II is essentially drawn directly from the review by Lhuillier and Misguich [49]. Our results show that, in this context at least, the term “quantum fluctuations” as discussed in the condensed matter literature can be identified precisely with entanglement as discussed in the quantum information literature, and the associated reduction of ground-state energy in antiferromagnets can be directly related to the theory of mixed state entanglement [37–39].

Note that the entanglement gap is well over a quarter of the total energy range for Heisenberg antiferromagnet on a line and is a very significant fraction of the total energy range for the majority of the lattices considered. This large entanglement gap reinforces the argument made by Brukner and Vedral [40] that the entanglement witnesses resulting from the energy of appropriate spin models can have macroscopic expectation values.

A. Bipartite lattices and mean-field theory

Mean-field theory is a term used to describe a variety of techniques in condensed matter physics for finding an approximation to the ground state of a quantum many-body system. Typically such techniques correspond to searching for a separable state that approximates the ground state. It is a well-known observation that mean-field theory is more accurate in higher dimensions and, because coordination number typically increases with the dimension, for higher coordination number. So, for example, dynamical mean-field theory for fermion systems is known to be exact in infinite dimensions [52].

In the context of our present work, we expect mean-field theory to work well when the entanglement gap is small, because there exists a separable state that has energy close to the ground-state energy and thus a variational approach involving separable states might be expected to be accurate. Theorem 3 demonstrates in a precise way that the entangle-

ment gap decreases to an arbitrarily small value with increasing coordination number on bipartite lattices, independent of the particular coupling Hamiltonian. This result is therefore suggestive of a quantitative connection between entanglement and the improvement of mean-field theory with dimension.

The work of Raggio and Werner [45] aimed to develop a rigorous mean-field theory for Hamiltonian models on star graphs with a large number of points. Our results are ultimately based on a characterization of bipartite separable states proven there and in Ref. [46], subsequently used in Ref. [44] to prove a result closely related to our Lemma 3. The proofs in Ref. [45] are technically very difficult, because they apply not only to finite-dimensional spin systems but to any quantum system defined on a separable Hilbert space. These results may provide a more direct route to our Theorem 2 for star-shaped graphs, which could then be used to prove the result for bipartite lattices in more generality; however, we have preferred to give a simple derivation valid for finite-dimensional spin systems.

B. Frustrated lattices and multipartite entanglement

Lattices that are not bipartite lead to spin systems that are often referred to as *frustrated* in condensed matter physics [53]. This terminology arises from the fact that the minimum-energy separable state for two neighboring sites on such a lattice is not equal to the minimum-energy separable for the two sites coupled alone. As a result the energy per bond on such a lattice is higher than the energy of a single pair for the same interaction.³ The physics of frustrated quantum and classical spin systems have been a subject of intensive research in recent years; we refer the reader to [53] for a review. In the following, we briefly consider the effect of frustration on the entanglement gap.

³Dawson and Nielsen [27] derive a bound on the ground-state entanglement based on the frustration of the *quantum* Hamiltonian, not the frustration of its classical counterpart.

Further motivation for studying lattices that are not bipartite comes from considering the nature of the entanglement detected by the Hamiltonian. On bipartite lattices, entanglement is only detected when the reduced density matrices associated with each bond are entangled. So, for example, states which are multipartite entangled but contain no bipartite entanglement, such as the three-party GHZ state, will never have lower energy than the minimum separable energy on a bipartite graph for any interaction Hamiltonian. On nonbipartite lattices it is sometimes possible for a coupling Hamiltonian to witness the entanglement of such states.

A simple example of a nonbipartite lattice is the regular triangular lattice, which is tripartite but not bipartite. We consider two other nonbipartite lattices in two dimensions: the kagomé lattice, which is made up of corner-sharing triangles, and the checkerboard lattice. These lattices are depicted in Fig. 1.

Again we consider the Heisenberg interaction. In order to find the lowest separable energy for the triangular and kagomé lattices, we first find a minimum-energy separable state for a single triangle, as described in Sec. III A. The total Hamiltonian for a single triangle is

$$H = \vec{\sigma}_1 \cdot \vec{\sigma}_2 + \vec{\sigma}_2 \cdot \vec{\sigma}_3 + \vec{\sigma}_3 \cdot \vec{\sigma}_1. \quad (31)$$

Its spectrum and minimum-energy separable states may be found by standard symmetry methods (for example, [54]). The ground state is fourfold degenerate with energy $E_0 = -3$. For the Heisenberg antiferromagnet of n spins with an all-to-all coupling, it is straightforward to show that a minimum-energy separable state is given by any configuration of spins where the total spin vector is zero [53]. For the triangle, a minimum-energy separable state is

$$|\uparrow\rangle_1 \otimes (|\uparrow\rangle_2 + \sqrt{3}|\downarrow\rangle_2)/2 \otimes (|\uparrow\rangle_3 - \sqrt{3}|\downarrow\rangle_3)/2, \quad (32)$$

which corresponds to a classical configuration of spins at an angle of $2\pi/3$ from each other in the plane having a total spin zero (the ‘‘Mercedes star’’ configuration in [54]). This state has energy $E_{\text{sep}} = -3/2$. The maximum-energy manifold is spanned by the states with all spins parallel and has energy $E_{\text{max}} = 3$.

From these results we can calculate the entanglement gap per bond and the scaled entanglement gap for the Heisenberg interaction on the triangle, shown in Table II. Also shown are the entanglement gaps for the kagomé and triangular lattices, calculated from E_{sep} for the triangle, and the ground-state energy of the entire lattice, taken from [49]. Note that, as for bipartite lattices, the entanglement gap per bond appears to decrease with coordination number. We have also considered the checkerboard lattice (see Fig. 1) which is made up of corner-sharing tetrahedra and has a coordination number of six. We obtain the ground-state energy of this model from Ref. [51], where it is estimated from exact diagonalization of small samples.

The reduced density matrices associated with bonds of the lattice in the ground state are not entangled for these frustrated systems. Note that the symmetries of the Heisenberg model guarantee that these bipartite reduced density matrices are so-called Werner states [55], invariant under any local unitary rotation of the form $U \otimes U$. These states are entirely

characterized by the fraction of the population that is in the singlet state, and when this fraction is less than a half, the state is separable [55]. Therefore the reduced density matrix associated with each bond is separable whenever the ground-state energy per bond is above the minimum separable energy of the Heisenberg Hamiltonian for a single pair of spins. With the ground-state energy per bond from Table II, it is clear that there is no bipartite entanglement of nearest-neighbor spins for the Heisenberg model on the triangular, kagomé, or checkerboard lattices (because E_0 per bond is greater than -1). The entanglement gap for these systems is associated with the entanglement of the reduced states of the triangles or tetrahedrons that make up the lattice. Thus, the Hamiltonian serves as a witness for multipartite entanglement in these systems.

It appears that as the frustration of the classical spin model increases, so does the entanglement gap. For a coordination number of 6 the entanglement gap as a fraction of the overall energy range of the Hamiltonian increases from 0.088 on the bipartite cubic lattice to 0.131 on the tripartite triangular lattice and finally to around 0.2 on the checkerboard lattice. It would be interesting to understand this behavior in more detail. It is a feature of frustrated classical spin models that they have a large number of configurations achieving the lowest possible energy, which may be a contributing factor to this observed larger entanglement gap.

C. Entanglement gap in a simple quantum phase transition

The role of entanglement in *quantum phase transitions* [11] is currently of considerable interest [4–6,10]. Perhaps the simplest model to exhibit a quantum phase transition, used in many of these studies, is the 1D infinite-lattice transverse field XY model with Hamiltonian

$$H = \sum_{j=0}^{N-1} \left(\frac{1+\gamma}{2} \sigma_j^x \sigma_{j+1}^x + \frac{1-\gamma}{2} \sigma_j^y \sigma_{j+1}^y + \lambda \sigma_j^z \right), \quad (33)$$

where γ is the anisotropy in the x - y plane, λ is an external magnetic field, N is the total number of lattice sites, and cyclic boundary conditions are imposed so that a subscript N is identified with 0. For $\gamma=1$ the transverse field Ising model is recovered.

It is of interest to see how this phase transition affects the entanglement gap. Here we calculate the entanglement gap of the 1D XY model as a function of (γ, λ) in the thermodynamic ($N \rightarrow \infty$) limit. Because a 1D lattice is bipartite (for N even), given knowledge of the ground-state energy it is sufficient to calculate the entanglement gap for the coupling Hamiltonian in order to calculate the entanglement gap of the entire system, as described in Sec. III. In this case the coupling Hamiltonian may be chosen to be

$$H_{ij}^{XY} = \frac{1+\gamma}{2} \sigma_i^x \sigma_j^x + \frac{1-\gamma}{2} \sigma_i^y \sigma_j^y + \frac{\lambda}{2} (\sigma_i^z + \sigma_j^z), \quad (34)$$

where the factor of $1/2$ in front of the magnetic field accounts for the fact that each site is involved in two interactions. In Appendix D we calculate the minimum separable

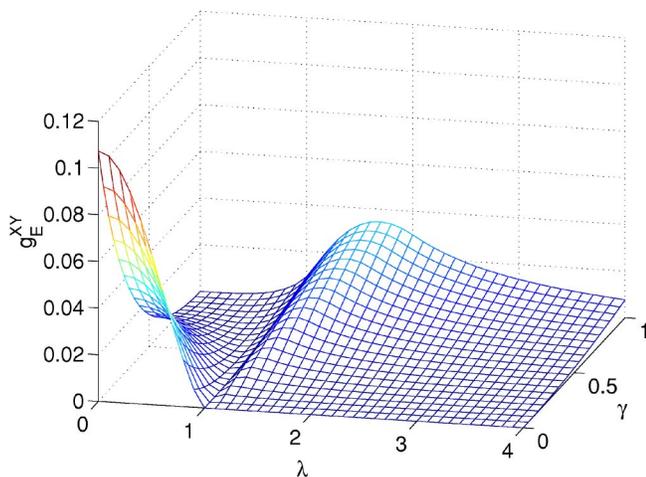


FIG. 2. Entanglement gap as a function of anisotropy γ and transverse field λ for XY Hamiltonian on a 1D lattice in the thermodynamic limit.

energy for this coupling Hamiltonian, Eq. (D4).

The XY model on a 1D chain, Eq. (33), is well known to be exactly solvable via the Jordan-Wigner transformation; see, e.g., [11]. We obtain the ground-state energy from this method.

In Fig. 2 we plot the scaled entanglement gap as a function of (γ, λ) in the thermodynamic limit. The quantum phase transition in this model occurs at $\lambda=1$ for $\gamma \neq 0$. Previous studies have indicated that the ground state becomes highly entangled at this point, and this behavior is manifest in a sudden rise in the entanglement gap about this point. Intuitively one might expect that the more entangled the ground state, the larger the entanglement gap. While qualitatively true, this connection cannot be exact because the entanglement gap is a property of the whole Hamiltonian; it can depend on all energy eigenstates and their energies and is not just a property of the ground state.

Nevertheless, given the discussion in Sec. II A it is reasonable to consider a connection between the ground-state entanglement as measured by $M(|\Psi\rangle)$ of Eq. (9) and the entanglement gap. The entanglement of the ground state under this measure has been investigated in the XY model in recent work by Wei *et al.* [8]. This measure depends only on the maximum overlap of the entangled state $|\Psi\rangle$ with a separable state. One might expect that the minimum-energy separable state is one which has the maximum overlap with the ground state. However, in order to achieve maximum overlap with the ground state it may also be necessary for a separable state to have large overlap with high-energy eigenstates. Therefore a separable state may achieve lower energy by having less overlap with the ground state but considerably more overlap with low-lying excited states.

In Ref. [8] the derivative of the global entanglement with respect to the external field was found to contain a singularity at the critical point consistent with the universality class of the model. Although we see a qualitatively similar peak near the critical point, there is no singularity in the derivative of the entanglement gap. Again, such a singularity may not have been expected because the entanglement gap is not simply a property of the ground state.

D. Summary

We have studied entanglement in quantum many-body systems from the point of view of the Hamiltonian as an entanglement witness. We introduced two related concepts useful in studying the role of entanglement in the ground and thermal states of multipartite quantum systems. The first is the entanglement gap, which is the difference in energy between the ground-state energy and the minimum energy that any separable state can attain. If the energy of the system lies within the entanglement gap range, the state of the system is guaranteed to be entangled. The second concept is the entanglement-gap temperature: the temperature at which the energy of the thermal state is equal to the minimum separable energy and below which the thermal state must be entangled. The entanglement-gap temperature provides a threshold for deducing the thermal state of the system to be entangled, based on its energy.

For multipartite, finite-dimensional quantum systems we proved that Hamiltonians possessing a nondegenerate maximally entangled ground state (according to a global measure of entanglement) and all other energy eigenstates degenerate maximize the entanglement gap. The related question of which Hamiltonians have the highest entanglement gap temperature is more challenging; substantial evidence is given that the Heisenberg antiferromagnetic Hamiltonian has the largest entanglement temperature for two qubits.

On bipartite lattices—i.e., those lattices for which there are only interactions between two disjoint subsets of the vertices—we proved that the entanglement gap decreases to zero as the coordination number increases. This result suggests a quantitative reason why approximation schemes based on separable states, such as various forms of mean-field theory, appear to give more reliable results at higher coordination number.

On frustrated lattices—i.e., those that are not bipartite—we noted that the Hamiltonian can act as an entanglement witness for multipartite entanglement, even when there is no bipartite entanglement present. Finally, we calculated the entanglement gap near a simple quantum phase transition and showed that, although it does not follow any universal scaling law, it does increase near the quantum phase transition, as may have been expected from previous studies in which the ground state was found to become highly entangled at that point.

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APPENDIX A: SEMIDEFINITE PROGRAMS FOR THE ENTANGLEMENT GAP

We will now describe efficient numerical procedures for evaluating the entanglement gap of a given Hamiltonian using semidefinite programs.

Semidefinite programs are a type of convex optimization problem [56,57], which are appealing because they have efficient numerical implementations. With the view of Hamil-

tonians as entanglement witnesses, and following methods described in [44,58,59] it is possible to express the problem of finding the minimum separable energy as a sequence of semidefinite programs, whose solutions converge to E_{sep} . The simplest program, which applies for bipartite systems with Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$, is

$$\begin{aligned} & \max \epsilon, \\ & \text{subject to } H - \epsilon I = P + Q^{T_A}, \\ & P \geq 0, \\ & Q \geq 0, \end{aligned} \quad (\text{A1})$$

where T_A denotes the partial transpose over system A . Let $d_i = \dim(\mathcal{H}_i)$, $i=A, B$. When $d_A=2$ and $d_B=2$ or 3 the maximum ϵ obtained from this program corresponds to the minimum separable energy E_{sep} . The optimum value ϵ^* of the semidefinite program gives an entanglement witness $Z_{EW} = H - \epsilon^* I$ and a lower bound on the entanglement gap equal to the largest magnitude negative eigenvalue of Z_{EW} . The entanglement witness produced by Eq. (A1) is referred to as *decomposable* because it can be written $Z_{EW} = H - \epsilon^* I = P + Q^{T_A}$ for $P \geq 0$, $Q \geq 0$ and can only detect entangled states with nonpositive partial transpose.

If the subsystems are of higher dimension, it is possible for an entangled state to have a positive partial transpose. Such states are *bound entangled* [60], and the semidefinite program (A1) only finds the gap between the ground-state energy and the minimum-energy positive partial transpose state. This solution provides a lower bound on E_{sep} , and it is possible to devise a nested sequence of programs that provide increasingly tighter bounds [44].

As all entanglement witnesses may be viewed as Hamiltonians with entangled low-energy states, one way of producing bound entangled states suggests itself: as thermal states. An example of a Hamiltonian for which there are bound entangled states which achieve lower energy than any separable state may be derived from the Choi form, as described in [44,60]. This Hamiltonian, which acts on the minimal-dimension system on which bound entangled states exist—i.e., $\dim(\mathcal{H}_A) = \dim(\mathcal{H}_B) = 3$ —is

$$\begin{aligned} H = & 2(|00\rangle\langle 00| + |11\rangle\langle 11| + |22\rangle\langle 22|) + |02\rangle\langle 02| + |10\rangle\langle 10| \\ & + |21\rangle\langle 21| - 3|\psi_+\rangle\langle \psi_+|, \end{aligned} \quad (\text{A2})$$

where $|\psi_+\rangle = (1/\sqrt{3})\sum_{i=0}^2 |ii\rangle$. The ground-state energy of this Hamiltonian is -1 , the minimum separable energy is 0, and there are bound entangled states with energy as low as $(3 - 2\sqrt{3})/3 \approx -0.1547$. Although $E_{\text{sep}} = 0$ the semidefinite program (A1) would return -0.1547 for this Hamiltonian, the energy of the minimum-energy positive partial transpose state. Implementing higher-order programs as per [44] would give more and more accurate estimates of the true minimum separable energy $E_{\text{sep}} = 0$. Furthermore, there is a small range of temperatures, $1.256 \leq k_B T \leq 1.271$, over which the thermal state has energy less than zero, so it is certainly entangled, but has positive partial transpose. Over this range of tem-

peratures the Hamiltonian witnesses the bound entanglement of the thermal state.

Examples of Hamiltonians where *all* low-energy states are bound entangled may be constructed from *unextendable product bases* [61]: a set of product states for which the orthogonal complement contains no product states. To construct the Hamiltonian we let the unextendable product basis span the excited-state manifold and its orthogonal complement the ground-state manifold. In this extreme example, all thermal states with energy within the entanglement gap are bound entangled.

APPENDIX B: ENTANGLEMENT-GAP TEMPERATURE OF BIPARTITE SYSTEMS

In this appendix, we investigate the entanglement-gap temperature of bipartite Hamiltonians. For this purpose, we define a *completely entangled* subspace of a multipartite Hilbert space as one that contains no separable states. The antisymmetric subspace of two systems is an example. One might wonder whether it is possible to find a Hamiltonian with a completely entangled ground-state manifold that is larger than the antisymmetric subspace so as to achieve a higher entanglement-gap temperature than the symmetric projector (18). In [62] the maximum dimension of a completely entangled subspace of many parties was investigated: for two d -dimensional systems a basis was given for a completely entangled subspace of maximum possible dimension $d^2 - 2d + 1$. This subspace contains the antisymmetric subspace.

A natural candidate for a Hamiltonian with a high entanglement-gap temperature is thus the Hamiltonian with such a subspace at energy zero and its orthogonal complement at the highest energy. To find its entanglement gap we could, in principle, use a sequence of semidefinite programs as described in Appendix A. However, as the dimension increases we need to implement increasingly higher-order tests to ensure convergence and computer memory requirements become prohibitive. These programs always return a *lower bound* on the entanglement gap. Alternatively, we can bound the gap from above by choosing random pure product states⁴ and evaluating their energies. The lowest energy of a large number of trial states provides an *upper bound* on the entanglement gap and thus on the entanglement-gap temperature.

Figure 3 compares the behavior of the entanglement gap temperature as a function of d for the three Hamiltonians considered above, $H_{\text{me}} = I - |\phi_d\rangle\langle \phi_d|$, $H_S = \Pi_S$, and $H_{\text{ces}} = I - \Pi_{\text{ces}}$, where Π_{ces} is the projector onto the completely entangled subspace of maximum dimension. We see that the entanglement-gap temperature of $H_{\text{ces}} = I - \Pi_{\text{ces}}$ is generally comparable to that of $H_{\text{me}} = I - |\phi_d\rangle\langle \phi_d|$. This result is due to the fact that the entanglement gap for H_{ces} is quite small, thus

⁴To create random pure quantum states we draw the components from $\mathcal{N}(0, 1)$ —i.e., a normal distribution with mean 0 and variance 1—and normalize the state. This sampling is equivalent to choosing states according to the Haar measure (see, for example, Appendixes A and B of Ref. [63]).

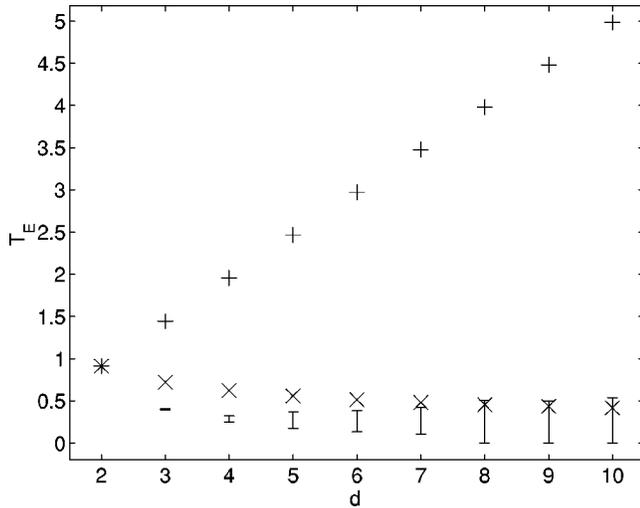


FIG. 3. Comparison of entanglement-gap temperature as a function of dimension of the subsystems for the three bipartite Hamiltonians: crosses correspond to $H_{me}=I-|\phi_d\rangle\langle\phi_d|$, pluses to $H_S=\Pi_S$, and bounding bars to $H_{ces}=I-\Pi_{ces}$.

resulting in low entanglement-gap temperature despite the large ground-state degeneracy.

Another method for constructing completely entangled subspaces is as the orthogonal complement of *unextendable product bases* [61]. We have constructed Hamiltonians with completely entangled ground-state manifolds from a number of known unextendable product bases and have always found entanglement-gap temperatures significantly lower than that of the symmetric-projector Hamiltonian.

We thus have good evidence that the symmetric-projector Hamiltonian has the highest entanglement-gap temperature of Hamiltonians with all energy eigenvalues either 0 or 1. The completely general case where there can be intermediate energies as well is beyond the scope of this work.

APPENDIX C: MAXIMUM ENTANGLEMENT-GAP TEMPERATURE FOR TWO QUBITS

In this appendix we investigate the entanglement temperature of two-qubit systems and provide evidence that the Heisenberg antiferromagnetic Hamiltonian has the highest scaled entanglement-gap temperature. We scale all two-qubit Hamiltonians so that the ground-state energy is 0, the maximum energy is 1, and there are two intermediate energies, $0 \leq E_1 \leq E_2 \leq 1$. The antiferromagnet has the singlet at energy 0 and all triplet states at energy 1; its scaled entanglement gap and entanglement-gap temperature are $g_E=1/2$ and $T_E=1/\log_e(3)$.

We present two lemmas leading to a theorem that any Hamiltonian with a maximally entangled ground state has an entanglement-gap temperature lower than that of the Heisenberg antiferromagnet.

Lemma 5. Let H and H' be two multipartite Hamiltonians with entanglement gap temperatures T_E and T'_E , respectively. If there is a separable state, ρ_{sep} such that

$$\text{tr}[H'\rho_{sep}] \leq U'(T_E), \quad (C1)$$

where $U'(T)$ is the thermal energy of H' , then $T'_E \leq T_E$.

Proof. $\text{tr}[H'\rho_{sep}]$ is an upper bound on $E'_{sep} = \min_{\rho_{sep} \in \mathcal{S}} \text{tr}[H'\rho_{sep}]$. By definition $U'(T'_E) = E'_{sep}$, so the result follows from the fact that $U'(T)$ is a monotonically increasing function of T . ■

Lemma 6. Any Hamiltonian H' with $E_1 \leq 1/4$ has an entanglement-gap temperature less than that of the Heisenberg antiferromagnet.

Proof. We use the fact that, for two qubits, all two-dimensional subspaces contain a separable state [62]. Thus, there must be a separable state in the subspace spanned by $|E_0\rangle$ and $|E_1\rangle$, and this separable state must have energy less than or equal to E_1 .

We now apply Lemma 5 with this separable state ρ_{sep} . Because E_1 is the lower of the two intermediate energies, the Hamiltonian H'' with the same eigenstates and eigenenergies as H' , except that $E_2=E_1$ will certainly have a lower thermal energy at any particular temperature than H' , $U''(T) \leq U'(T)$, $\forall T$. The thermal energy $U''(T)$ is easily calculated; with it, we find a value of E_1 that satisfies the condition

$$E_1 \leq U''(T_E = 1/\log_e(3)) \Rightarrow E_1 \leq 1/4. \quad (C2)$$

Thus, if $E_1 \leq 1/4$, then $\text{tr}[H'\rho_{sep}] \leq U''(T_E = 1/\log_e(3)) \leq U'(T_E = 1/\log_e(3))$, so H' has a lower entanglement-gap temperature than the Heisenberg antiferromagnet, as required. ■

Theorem 4. Any Hamiltonian H' with a maximally entangled ground state has an entanglement-gap temperature less than that of the Heisenberg antiferromagnet.

Proof. Given a Hamiltonian with a maximally entangled ground state we can use local unitaries to transform to a Hamiltonian with the singlet as its ground state $|E_0\rangle = (|0\rangle|1\rangle - |1\rangle|0\rangle)/\sqrt{2}$. By Lemma 1 and the invariance of the spectrum under any unitary, this Hamiltonian has the same entanglement-gap temperature. The excited eigenstates for this Hamiltonian all lie in the symmetric (triplet) subspace. We express the excited states in their Schmidt decompositions as $|E_i\rangle = \lambda_i|0_i\rangle|0_i\rangle + \sqrt{1-\lambda_i^2}|1_i\rangle|1_i\rangle$, where $i=1, 2, 3$.

We present two separable states, one of which has energy less than the threshold for any Hamiltonian. The first is $\rho_{sep} = |A\rangle\langle A| \otimes |B\rangle\langle B|$ where

$$|A\rangle = (|0_1\rangle + |1_1\rangle)/\sqrt{2}, \quad |B\rangle = (|0_1\rangle - |1_1\rangle)/\sqrt{2}. \quad (C3)$$

The energy of this state is at most $\text{tr}[H'\rho_{sep}] = (E_1+1)/4$. For a given E_1 this energy will be less than $U'(T_E)$ for E_2 greater than a certain lower bound, E_2^{lb} . $E_2^{lb}(E_1)$ is defined implicitly by

$$\text{tr}[H'\rho_{sep}] = U'(T_E = 1/\log_e(3)). \quad (C4)$$

This equation is transcendental and so it is not possible to find an explicit functional form for $E_2^{lb}(E_1)$.

The second low-energy separable state that we consider is $\rho_{sep} = |A\rangle\langle A| \otimes |B\rangle\langle B|$ where $|A\rangle = |0_3\rangle$ and $|B\rangle = |1_3\rangle$. The energy of this state is at most $\text{tr}[H'\rho_{sep}] = E_2/2$. This energy will be less than $U'(T_E = 1/\log_e(3))$ for E_2 less than a maximum value $E_2^{ub}(E_1)$, defined by

$$E_2/2 = U'(T_E = 1/\log_e(3)). \quad (C5)$$

We numerically solve the two equations (C4) and (C5) for $E_2^{lb}(E_1)$ and $E_2^{ub}(E_1)$, respectively. From Lemma 5 it is only possible that $T'_E > T_E = 1/\log_e(3)$ if $E_1 > 1/4$. However, it is straightforward to calculate numerically $E_2^{lb}(E_1) \leq E_2^{ub}(E_1)$ in this region, so that for any (E_1, E_2) , there is a separable state with energy less than $U'(T_E = 1/\log_e(3))$. Lemma 6 requires that $T'_E \leq T_E$, so the Heisenberg antiferromagnet has the highest entanglement-gap temperature of any bipartite Hamiltonian with a maximally entangled ground state. ■

A generic two-qubit Hamiltonian has a nonmaximally entangled ground state, so it is still possible that such a Hamiltonian possesses a higher entanglement-gap temperature than the Heisenberg antiferromagnet. To provide numerical evidence that such a Hamiltonian does not exist, we generated random Hamiltonians by drawing the two intermediate energy levels from a uniform distribution. Because no bound entangled states exist for two qubits, the semidefinite program of Appendix A produces the entanglement gap. We then calculated the entanglement-gap temperature numerically. We generated 10^8 random Hamiltonians and calculated their entanglement-gap temperature in this way. None were found to have an entanglement-gap temperature higher than that of the Heisenberg antiferromagnet, providing strong evidence that it possesses the highest possible entanglement-gap temperature.

APPENDIX D: TRANSVERSE FIELD XY MODEL

The transverse field XY model is defined by the coupling Hamiltonian, Eq. (34). To find the minimum-energy separable state $|A\rangle|B\rangle$ we parametrize the two factors as

$$|j\rangle = \cos \theta_j |\uparrow\rangle + e^{i\phi_j} \sin \theta_j |\downarrow\rangle, \quad j = A, B, \quad (D1)$$

where $0 \leq \theta_j \leq \pi/2$, $0 \leq \phi_j < 2\pi$. We then calculate the energy of the product state $|A\rangle|B\rangle$ as a function of the four parameters:

$$\begin{aligned} \langle A | \langle B | H_{AB}^{XY} | A \rangle | B \rangle &= \frac{\lambda}{2} (\cos 2\theta_A + \cos 2\theta_B) \\ &+ \left(\frac{1+\gamma}{2} \right) \cos \phi_A \sin 2\theta_A \cos \phi_B \sin 2\theta_B \\ &+ \left(\frac{1-\gamma}{2} \right) \sin \phi_A \sin 2\theta_A \sin \phi_B \sin 2\theta_B, \end{aligned} \quad (D2)$$

and optimize over this space to find the lowest-energy separable state. The result is

$$|j\rangle = \begin{cases} \sqrt{\frac{1+\gamma+\lambda}{2(1+\gamma)}} |\uparrow\rangle \pm \sqrt{\frac{1+\gamma-\lambda}{2(1+\gamma)}} |\downarrow\rangle, & \lambda \leq 1+\gamma, \\ |\downarrow\rangle, & \lambda \geq 1+\gamma, \end{cases} \quad (D3)$$

where the \pm corresponds to $j=A, B$, with energy

$$E_{\text{sep}}^{XY} = \begin{cases} -\frac{(1+\gamma)^2 + \lambda^2}{2(1+\gamma)}, & \lambda \leq 1+\gamma, \\ -\lambda, & \lambda \geq 1+\gamma. \end{cases} \quad (D4)$$

Incidentally, by calculating the spectrum of H_{AB}^{XY} we can identify a curve $\lambda^2 + \gamma^2 = 1$ on which there is a separable state in the degenerate ground-state manifold. The entanglement gap is therefore zero on this curve, and this result remains true for the XY model on an arbitrary bipartite lattice (with the appropriate magnetic field in the coupling Hamiltonian).

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